



THE UNIVERSITY *of* EDINBURGH

## Edinburgh Research Explorer

### Embrittlement and the bistable crystal structure of zirconium hydride - Ackland replies

**Citation for published version:**

Ackland, GJ 1998, 'Embrittlement and the bistable crystal structure of zirconium hydride - Ackland replies', *Physical Review Letters*, vol. 81, no. 15, pp. 3301-3301. <https://doi.org/10.1103/PhysRevLett.81.3300>

**Digital Object Identifier (DOI):**

[10.1103/PhysRevLett.81.3300](https://doi.org/10.1103/PhysRevLett.81.3300)

**Link:**

[Link to publication record in Edinburgh Research Explorer](#)

**Document Version:**

Publisher's PDF, also known as Version of record

**Published In:**

Physical Review Letters

**General rights**

Copyright for the publications made accessible via the Edinburgh Research Explorer is retained by the author(s) and / or other copyright owners and it is a condition of accessing these publications that users recognise and abide by the legal requirements associated with these rights.

**Take down policy**

The University of Edinburgh has made every reasonable effort to ensure that Edinburgh Research Explorer content complies with UK legislation. If you believe that the public display of this file breaches copyright please contact [openaccess@ed.ac.uk](mailto:openaccess@ed.ac.uk) providing details, and we will remove access to the work immediately and investigate your claim.



## Embrittlement and the Bistable Crystal Structure of Zirconium Hydride

In a recent Letter [1] Ackland proposed that the delayed hydride cracking (DHC) in zirconium alloys can be attributed to a mechanical instability of the cubic phase in an external strain field with respect to a tetragonal distortion, which leads to uniaxial misfit strains and causes DHC. This suggestion is based on *ab initio* electronic structure calculations using norm-conserving nonlocal pseudopotentials carried out for cubic fluorite structure  $\text{ZrH}_2$  and for tetragonal distortion of the cubic cell over a range of values of the  $a$  and  $c$  parameters. He finds that  $\text{ZrH}_2$  is an insulator in both the cubic and tetragonal phases. This result is in complete contradiction with both theoretical calculations [2–4] which are not cited in Ackland's Letter and experimental data which include electronic specific heat [5,6], magnetic susceptibility [6,7], thermoelectric power [6,8], and nuclear magnetic resonance [9–11], where  $\text{ZrH}_2$  is found to be metallic.

To confirm this contradiction, we have performed new band structure calculations for  $\text{ZrH}_2$  in both cubic

and tetragonal forms ( $c/a = 0.893$ ) within the local density approximation (LDA) using the linear muffin-tin orbital in the atomic sphere approximation method with combined correction terms. The total densities of states (DOS) calculated using the linear energy tetrahedron method are plotted in Fig. 1 for the cubic and tetragonal structures. In agreement with previous LDA calculations [2–4], the zirconium dihydrides are characterized by two low-energy bands due to metal-hydrogen bonding and H-H interactions. These bands which correspond to the two peaks in the DOS observed below  $-4$  eV in Fig. 1 overlap the Zr- $d$  states extending above  $-4$  eV. The Fermi energy  $E_F$  of cubic  $\text{ZrH}_2$  is located on a peak of high DOS which is associated with a dispersionless doubly degenerate band in the  $[111]$   $\Gamma L$  direction of the fcc Brillouin zone. This degeneracy is lifted by the tetragonal distortion leading to a decrease of the DOS at  $E_F$  in the tetragonal phase; this result is in agreement with suggestions based on experimental observations [5–11] and previous calculations [2–4]. The hydrides in the two phases are clearly metallic. The DOSs obtained by LDA calculations bear no common features with those plotted by Ackland in Fig. 3 of his Letter. A close examination of Fig. 1 of Ackland's Reply shows that this figure is not simply "a backward tracing" of Fig. 3 of his Letter. We therefore believe that there is a serious mistake in his band structure calculations which invalidates his suggestions concerning embrittlement and DHC in zirconium.

M. Gupta

Institut des Sciences des Matériaux, L.E.M.H.E.  
Bâtiment 415, Université Paris-Sud  
91405-Orsay, France

Received 2 April 1998

[S0031-9007(98)07395-5]

PACS numbers: 81.40.Np, 61.50.Ah, 62.20.Dc

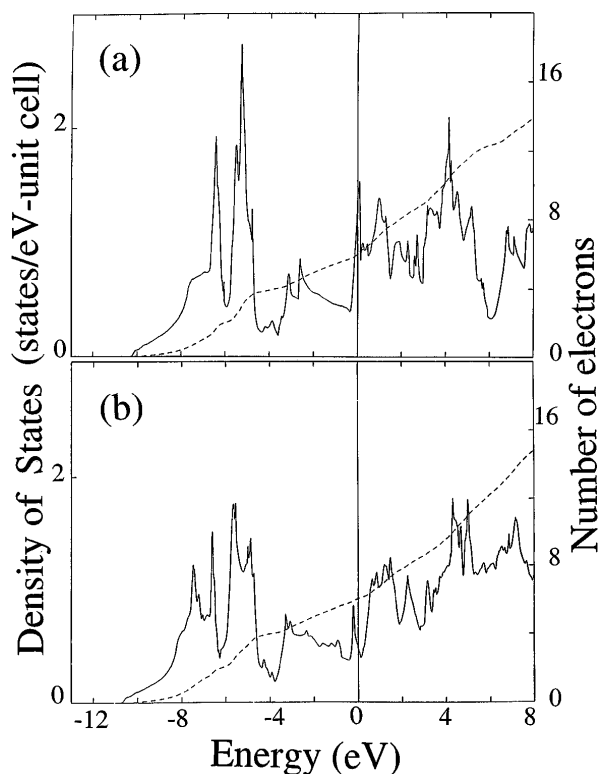


FIG. 1. The total densities of states (full curve) and the number of electrons (dashed curve). The Fermi energy is chosen as the origin: (a) cubic  $\text{ZrH}_2$ ; (b) tetragonal  $\text{ZrH}_2$ .

- [1] G. J. Ackland, Phys. Rev. Lett. **80**, 2233 (1998).
- [2] A. C. Switendick, J. Less-Common Met. **49**, 283 (1976); **103**, 309 (1984).
- [3] D. A. Papaconstantopoulos and A. C. Switendick, J. Less-Common. Met. **103**, 317 (1984).
- [4] M. Gupta and L. Schlapbach, in *Hydrogen in Intermetallic Compounds I*, Topics in Applied Physics Vol. 1, edited by L. Schlapbach (Springer-Verlag, Berlin, 1988), p. 139.
- [5] K. Bohmhammel *et al.*, J. Low Temp. Phys. **43**, 521 (1981).
- [6] F. Ducastelle *et al.*, J. Phys. (Paris) **31**, 57 (1970).
- [7] H. Nagel and H. Goretzki, J. Phys. Chem. Solids **36**, 431 (1975).
- [8] K. Gesi *et al.*, Nucl. Metall. **10**, 4 (1964).
- [9] R. Göring *et al.*, J. Phys. C **14**, 5675 (1981).
- [10] R. C. Bowman, Jr. *et al.*, Phys. Rev. B **27**, 1474 (1983).
- [11] C. Korn, Phys. Rev. B **28**, 95 (1983).